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Excitation of Hydrogen Molecules by

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- Excitation to $D(3p\pi^1\Pi_{11})$ State -

by

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ABSTRACT

The investigation of the excitation of the hydrogen molecule by electron impact, employing one-center wave functions and Born and Born-Ochkur approximations, has been extended to the $D(3p\pi^1\Pi_{11})$ excited state (the excitation to the B and C states of the hydrogen molecule has been recently investigated by the author elsewhere). The oscillator strength is in excellent agreement with the experimental value of Geiger and with the theoretical value of Mulliken and Rieke. However, the generalized oscillator strength are larger for $K < 0.33$ and smaller for higher values of K than those obtained by Roscoe. The total excitation cross sections are in fair accord with the estimates of Craggs and Massey.

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Recently the excitation of the hydrogen molecule from the ground state $X(1s\sigma^2 \Sigma_g^+)$ to the excited states $B(2p\sigma^2 \Sigma_u^+)$ and $C(2p\pi^2 \Pi_u)$ by electron impact, employing one-center wave functions of Huzinaga¹ and Born and Ochkuř² approximations, has been investigated by the author³. Fair agreement between the theoretical values and the experimental results of Geiger⁴ has been obtained. The experimental investigation of Geiger also includes the $D(3p\pi^2 \Pi_u)$ state of the molecule and his results show that the optical oscillator strength of the D state is about 25 % higher than to be expected from the theoretical investigation of Roscoe⁵ who employed multi-center wave functions and the integrals have been evaluated only approximately. Hence it is of interest to extend the investigation, using one-center wave functions which are expected to be more accurate for higher excited states, to the excitation of the molecule to the D state.

Following the notations of Paper I, for the one-center wave function of the D state we have⁶

$$\Psi_D(r_1, r_2, R) = \frac{1}{\sqrt{2}} \left[\phi_{in}^D(r_1) \phi_{out}^D(r_2) + \phi_{in}^D(r_2) \phi_{out}^D(r_1) \right] \quad (1)$$

Where the position vectors \underline{r}_1 and \underline{r}_2 of the molecular electrons are being referred to the center of the molecule, R is the internuclear distance, $\phi_m^D(r)$ is the same as $\phi_m^{B.C.}(r)$ of Paper I but $\phi_{out}^D(r)$ is modified to

$$\phi_{out}^D(r) = \frac{(2\gamma_2^D)^{1/2}}{\sqrt{6!}} r^2 e^{-\gamma_2^D r} \frac{1}{\sqrt{2}} (\gamma_{11} + \gamma_{12}) \quad (2)$$

Where Y_{lm} are normalized spherical harmonics. A variational calculation for E_D , the energy of the D state, at $R = 1.4$, the equilibrium internuclear distance of the ground state, yields $\eta_2^D = 0.338$ and $E_D = -0.605660$. Taking $E_0 = -1.120566^1$, the energy of the ground state, we obtain the threshold of the excitation potential for the D state to be 14.0 eV, which seems to be a reasonable value⁴. It may be noted that η_2^D is quite close to $\frac{1}{3}$ hence for higher excited states it should be a satisfactory assumption to take η_2 equal to $\frac{1}{n}$ where n is the principal quantum number of the excited electron.

For better comparison we have reduced the differential cross sections given by Roscoe⁵ to the generalized oscillator strength using (10) of Paper I and 14 eV for the excitation potential. Figure 1 shows that the present values of the generalized oscillator strength are larger for $K < 0.33$ and are smaller for higher values of K than those obtained by Roscoe⁵.

The difference between the two sets of values is more pronounced for higher values of K . Unfortunately, no experimental data exists for comparison. However, the present value of the optical oscillator strength, which is equal to 0.052, is in excellent agreement with the Geiger's⁴ experimental value of 0.049 ± 0.007 . It also coincides with the theoretical value given by Mulliken and Rieke⁷ where two-center atomic orbital wave functions with effective nuclear charge equal to unity for all orbitals have been used. Figure 2 shows that the effect of exchange is to reduce the total excitation cross sections but the effect is small throughout which is similar to the excitation of the hydrogen molecule to the B and C states³. Further we notice that the total excitation cross sections are in fair accord with the estimates of Craggs and Massey⁸. However, it may be pointed out that the differential cross sections and the threshold of excitation potential used by Craggs and Massey are different from the present values.

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References and Footnotes

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Figure Captions

Figure 1 - The generalized oscillator strength for the excitation of the ground state hydrogen molecule by electron impact to the D electronic state:

A - present, B - Roscoe⁵, Φ and X denote the experimental and the theoretical values of the optical oscillator strength obtained by Geiger⁴ and Mulliken and Reike⁷ respectively.

Figure 2 - Total cross sections for the excitation of the ground state hydrogen molecule to the D electronic state by electron impact: D - Born Approximation; E - Born-Ochkur Approximation; F - Born cross section estimated by Craggs and Massey⁸ from the differential cross sections of Roscoe⁵.

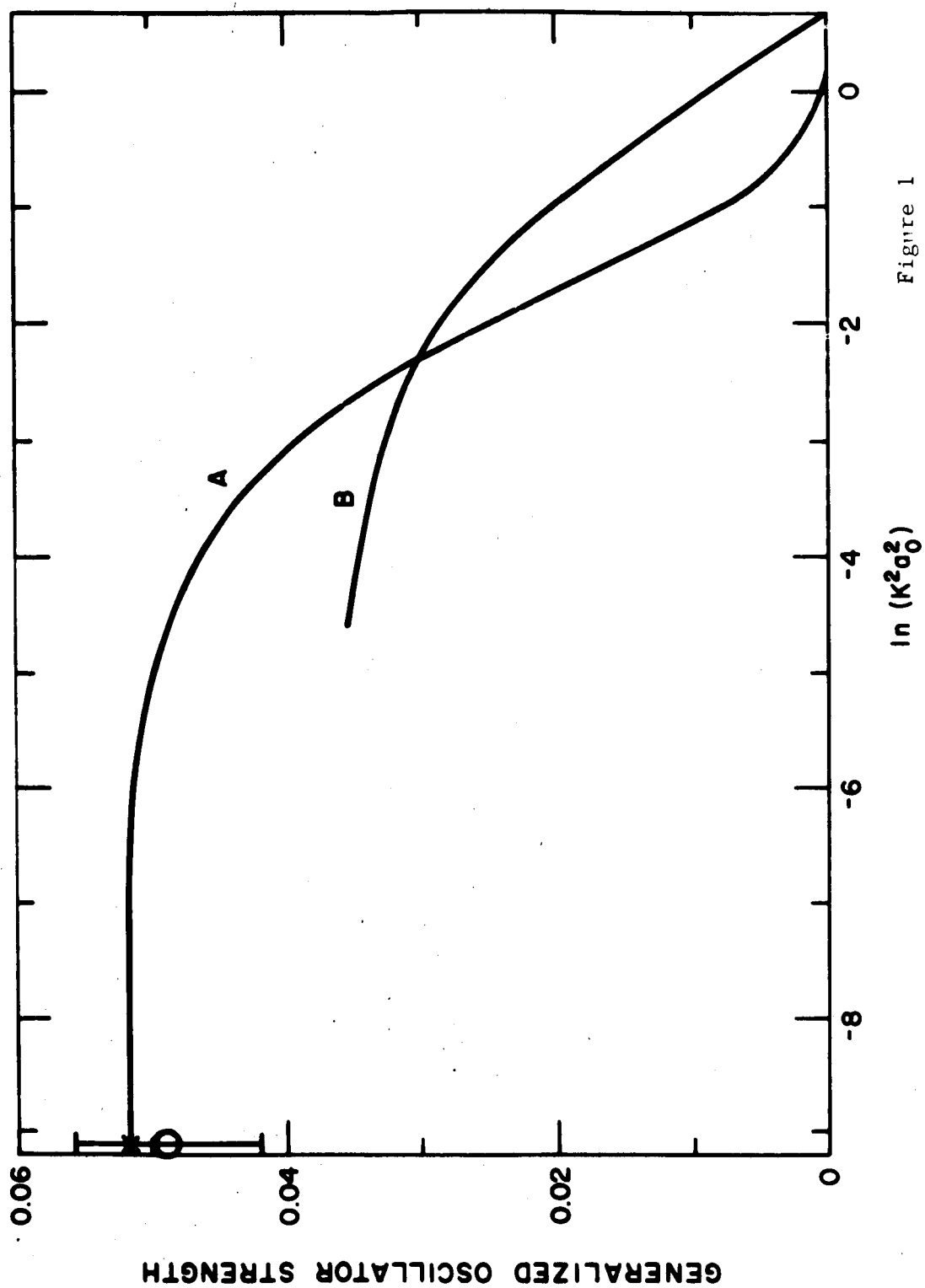


Figure 1

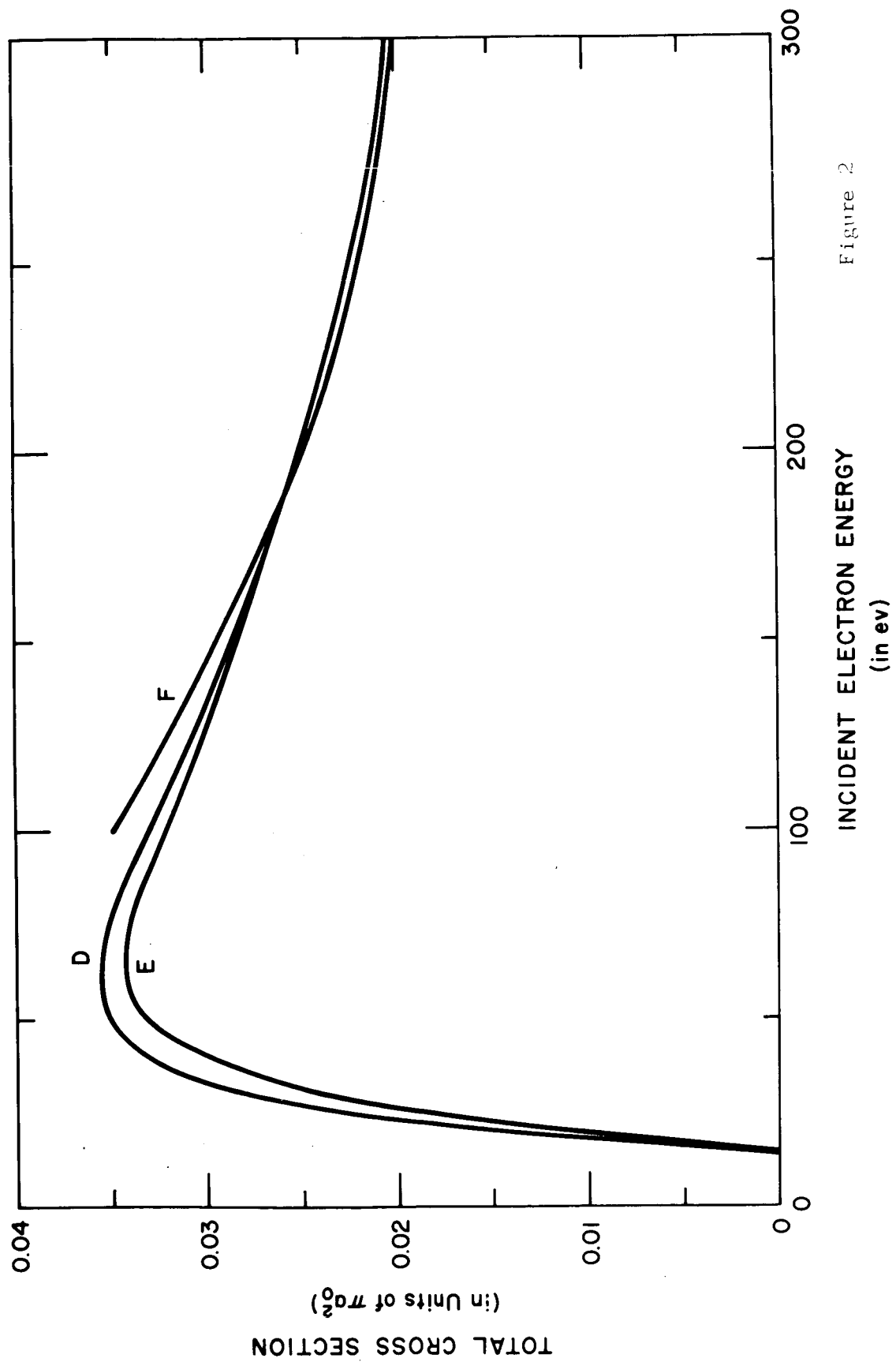


Figure 2